OMNIITOX: Opening

OMNIITOX Concept Model Supports Characterisation Modelling for Life Cycle Impact Assessment

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Abstract

Goal Scope Background. The main focus in OMNIITOX is on characterisation models for toxicological impacts in a life cycle assessment (LCA) context. The OMNIITOX information system (OMNIITOX IS) is being developed primarily to facilitate characterisation modelling and calculation of characterisation factors to provide users with information necessary for environmental management and control of industrial systems. The modelling and implementation of operational characterisation models on eco and human toxic impacts requires the use of data and modelling approaches often originating from regulatory chemical risk assessment (RA) related disciplines. Hence, there is a need for a concept model for the data and modelling approaches that can be interchanged between these different contexts of natural system model approaches.

Methods. The concept modelling methodology applied in the OMNIITOX project is built on database design principles and ontological principles in a consensus based and iterative process by participants from the LCA, RA and environmental informatics disciplines.

Results. The developed OMNIITOX concept model focuses on the core concepts of substance, nature framework, load, indicator, and mechanism, with supplementary concepts to support these core concepts. They refer to the modelled cause, effect, and the relation between them, which are aspects inherent in all models used in the disciplines within the scope of OMNIITOX. This structure provides a possibility to compare the models on a fundamental level and a language to communicate information between the disciplines and to assess the possibility of transparently reusing data and modelling approaches of various levels of detail and complexity.

Conclusions. The current experiences from applying the concept model show that the OMNIITOX concept model increases the structuring of all information needed to describe characterisation models transparently. From a user perspective the OMNIITOX concept model aids in understanding the applicability, use of a characterisation model and how to interpret model outputs.

Recommendations and Outlook. The concept model provides a tool for structured characterisation modelling, model comparison, model implementation, model quality management, and model usage. Moreover, it could be used for the structuring of any natural environment cause-effect model concerning other impact categories than toxicity.

Keywords: Characterisation model; concept model; informatics; information system; OMNIITOX

1 The Need for a Concept Model and System Requirements in OMNIITOX

The OMNIITOX project is of a multidisciplinary nature. Life cycle assessment (LCA) practitioners, chemical regulatory risk assessment (RA) expertise, as well as expertise from industry, academia, and government bodies are all foreseen to make use of the project results (Molander et al., this edition). Different users have different needs and can use different terminology for the same or related concepts. The task at hand is to facilitate efficient and understandable communication of information in this versatile user environment.

The main focus in OMNIITOX is on characterisation models in an LCA context, and the OMNIITOX information system (OMNIITOX IS) is being developed primarily to facilitate toxicological characterisation modelling and calculation to provide users with information necessary to manage and control industrial systems towards sustainability [1]. The modelling and implementation of operational characterisation models on eco and human toxic impacts developed in OMNIITOX require the usage of data and modelling approaches originating from the RA and related disciplines [2]. The ISO 14040 standard series provides a framework of concepts and terms suitable for LCA, but there is an additional need of a framework where data is consistently interchanged between contexts of natural system modelling approaches. The implementation of an information system puts specific requirements on the structuring of information as it is communicated between users via the technical and organisational components of the OMNIITOX IS. The terminology must not only be understandable by humans, but also translatable into a language interpretable by computers.

A concept model is a collection of named and described concepts including their relations. The OMNIITOX concept model is intended to support the structuring of natural system models for industrial applications in general and for operational characterisation models in particular. Moreover, it should describe the meaning of all types of information that are used by all parts – humans and technical components – interacting in and with the OMNIITOX IS. In this way, the concept model can serve as an essential support in characterisation modelling, model comparison, model implementation, model quality management, and model usage as information is communicated between the components inside the OMNIITOX IS and between external data sources and receivers [3].

2 Concept Modelling Methodology Applied in OMNIITOX

In OMNIITOX, a consensus based concept modelling methodology has been applied as the basis for developing the required multidisciplinary communication platform. The methodology also builds on the six database design principles as set up by Elmasri and Nanthe [4].

1. Requirement collection and analysis
2. Conceptual database design
3. Choice of Database Management system (DBMS)
4. Data model mapping
5. Physical database design
6. Database implementation

The first step – requirement collection analysis – concerned the definition of the scope and required functionality of the OMNIITOX IS. The participating organisations in the project are a cross-section of the intended users of the OMNIITOX IS with representatives of LCA practitioners, RA, as well as expertise from industry, academia, and government. In addition, the international character of the OMNIITOX consortium adds the aspect of cultural and lingual differences also within disciplines. It has therefore been a crucial aim to give all participants the opportunity to contribute with their needs, ideas, and terminologies.

In the second step – Conceptual database design – the analysis and the synthesis of the result from the first step were taken further to find a suitable concept model. In practice, this involved finding the essence in the field of study by analysing intersections and differences of related concepts used in the different disciplines. Initially a quite complex picture arises with ambiguities between the meanings of abstractions from different disciplines. Ontological principles are applied in order to create an understandable structure that sorts out what really is the object of study, i.e. the concept modelling aims at structuring information based on the physical causality found in the real world. The modelling has also applied the general design principles as described in the PHASENS model [5,6] to provide a baseline for model transparency and consistency. PHASENS – PHASEs in the design of a model of a Nature System – describes how information about changes in the natural systems (not being controlled by humans) are communicated and analysed. Additional important inputs to the concept modelling have been existing model frameworks including the toxicity impact assessment framework as described by SETAC working groups on impact assessment [7], as it has provided understanding of the state of the art in toxicity impact assessment modelling.

Step 1 and 2 was iterated until a first prototype version of the concept model was achieved. The information system developers in the OMNIITOX project performed the analysis and compilation, and the resulting concept model was presented.

In order to make the concept model interpretable by computers, the process continued by implementing the prototype concept model in a database through step 3–6. The Database Management System (DBMS) chosen is relational databases R-DBMS. This choice was made prior to the concept modelling process and was based on the fact that relational databases are a well established and well understood standard technology DBMS [8]. It is tested in a vast number of applications, and previous experiences have shown the high applicability of R-DBMS in environmental information management [9–12]. At the fourth step, the prototype concept model was transformed into a relational data model where entities and relations are translated into tables, primary keys, and foreign keys. The relational data model was written down as Structured Query Language (SQL) statements in step five. In the final step, the database objects were created by executing the SQL statements through the R-DBMS.

This overall process – step 1 to 6 – has been iterated until the user requirements are incorporated and the concept model follows R-DBMS rules. In this way, the OMNIITOX data format and the OMNIIITOX database were created simultaneously as the concept model was developed. The understanding and acceptance of the concept model has also increased in the iterative consensus process.

3 The Core of the OMNIITOX Concept Model

The design of the OMNIITOX concept model is based on the fact that a cause, an effect, and the relation between them within a defined system frame can be identified for all types of models of the natural system used in industrial applications. The concepts load, indicator, mechanism, nature framework, and substance are the cornerstones in the OMNIITOX concept model (**Fig. 1**). The arrows indicate relational dependency: an arrow that points from A to B means that A is dependent on B and requires the existence of B. In addition B is independent on A. The concepts load, indicator, substance, and nature framework are independent of other concepts, whereas mechanism requires the existence of the other four concepts. This is a key to the information structure of a cause effect model as it is not possible to define the relation between a cause and an effect without first defining what the cause and effect is. In addition to the core concepts, a number of concepts have been defined to support the core. This includes the structuring of substance property and nature property data, quality meta-data, units, reference documentation, mechanism algorithm, etc. A detailed description of the OMNIITOX concept model can be found in the OMNIITOX concept model and data format report [13].

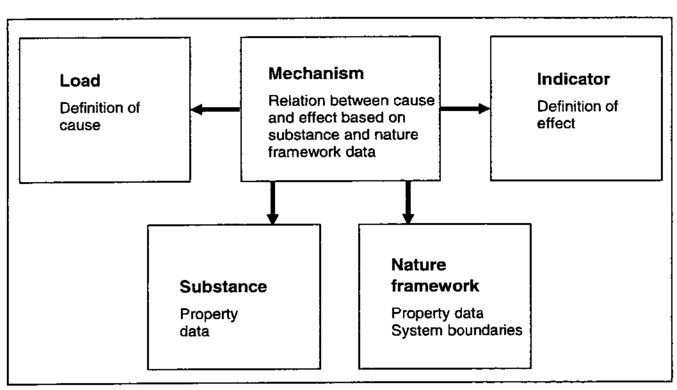

Fig. 1: The core of the OMNIITOX concept model. The arrows indicate relational dependency

3.1 Substance and nature framework

In OMNIITOX, a substance consists of physical matter, which can be an element, a chemical, a compound, a material, etc. A substance can be viewed in various contexts, such as in an emission quantity in an LCA study, or in a concentration in the natural system. However, the context in which a substance is viewed is not an intrinsic property of a substance. Substances have substance properties e.g. mass, colour, dissociation constant, degradability, acute toxicity to fish, etc. Definitions of substance properties are called substance property specifications. Measured data are connected to a substance and a property specification as a substance property value. The value may be dependent on conditions such as the temperature at the measurement. **Fig. 2** shows relations between substance property data.

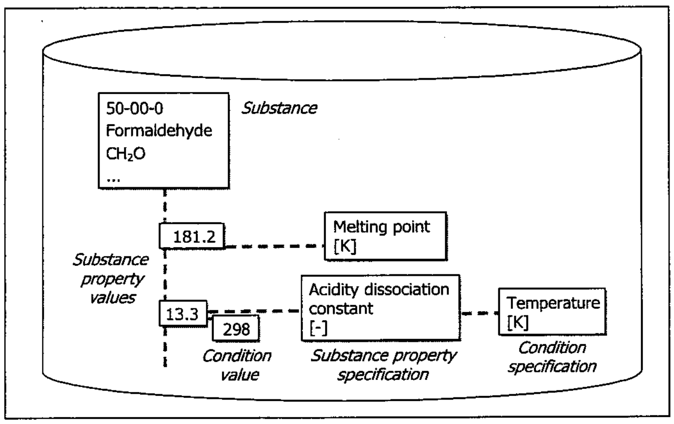

Fig. 2: Example of substance property data. A substance property value is defined by referring a substance and a substance property specification. In this case the substance with the names 50-00-0, Formaldehyde, and CH_2O is connected to the substance properties Melting point and Acidity dissociation constant

The nature framework concept refers to system frame models of the environment. Nature frameworks have system boundaries and properties that are independent of substances such as geographical location, wind speed, time of rain period, etc. These properties are called nature properties in the OMNIITOX concept model. Concepts for nature framework data are nature property specifications and nature property values in equivalence to substance, as shown in **Fig. 3**.

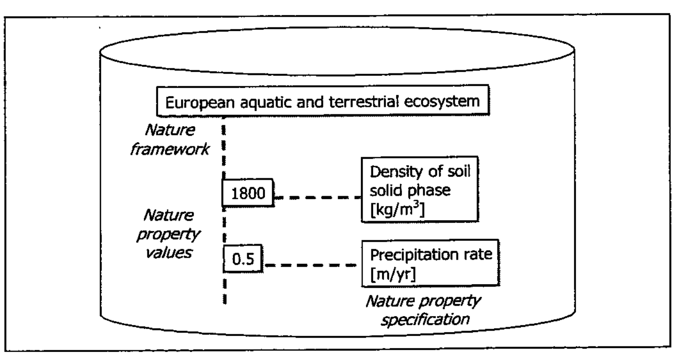

Fig. 3: A nature property value is defined by referring a nature framework and a nature property specification. In this example the nature framework named European aquatic and terrestrial ecosystem is connected to the nature properties Density of solid phase soil and Precipitation rate

3.2 Load and indicator

The load concept refers to the cause, i.e. what is considered to trigger the mechanism and in turn has an impact on an indicator. The load is independent of the mechanism as the same load may trigger many mechanisms. By just looking at the load, a specific mechanism cannot be distinguished. An example of a load definition is shown in **Fig. 4**.

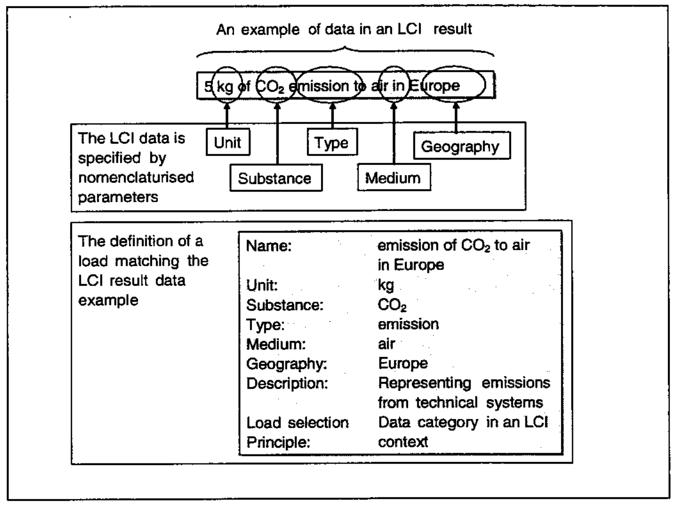

Fig. 4: Example of a load definition based on nomenclaturised parameters that matches LCI result data

An indicator is a quantifiable entity of interest within the nature system. In a cause-effect model the indicator is the definition of the effect. In the same way as for a load, an indicator is independent of any mechanism. Many mechanisms may affect the same indicator, and it is not possible, by just looking at the indicator, to distinguish which specific mechanism may affect it. The indicator is nevertheless defined for a specific reason. The impact indication principle, i.e. the reason why and the policy applied when an indicator is chosen must therefore be stated with the definition of the indicator. An example of an indicator definition is shown in **Fig. 5**.

It is important to distinguish the definitions of loads and indicators from values of loads and indicators. Loads and indicators only define the domains of valid load values and indicator values.

Example of an indicator definition

Name:	Concentration of formaldehyde in fresh water compartment in Europe
Unit:	kg/m³
Substance:	Formaldehyde
Medium:	Fresh water
Geography:	Europe
Description:	Representing increase of concentration over background of formaldehyde in fresh water compartment in Europe
Impact Indication Principle:	ERA fate modelling principles

Fig. 5: Example of an indicator definition

3.3 Mechanism

Once the load and indicator are defined in a cause effect chain model the relation between them can be defined. The mechanism concept refers to this relation. It determines the magnitude of the impact on an indicator due to the load. This relation is based on a defined set of substance and nature properties. The system boundaries of the nature framework also define system frame of the mechanism. In this way the mechanism model connects the other independent core concepts together. One or several loads and indicators may be referred to by the same mechanism. A descriptive explanation of the mechanism is required as well as a mathematical definition of any algorithms applied. In a linear characterisation model the mechanism is mathematically expressed as characterisation factors, see Chapter 4.

3.4 Comparison with related concepts

The core concepts represent key elements of a rich language and point out the common denominators of modelling approaches in relevant disciplines. In characterisation models in LCA, toxicological measurements, exposure and effect assessment in RA methodology, it is possible to distinguish the core concepts. Internally, the different modelling approaches use different concepts with slightly different meaning as exemplified in **Table 1**. By structuring the data of these models according to the OMNIITOX concept model, it is possible to consistently compare numeric outputs of models and it provides possibilities to assess the reusability of data and modelling methodology.

3.5 Comparison with SETAC framework

The SETAC Europe's First Working Group on Life Cycle impact assessment (WIA1) proposed a framework for ecotoxicity and human toxicity characterisation within life cycle impact assessment (LCIA) [7], in the following text referred to as the SETAC framework. The SETAC framework builds on experiences primarily from RA and contains many aspects relevant to OMNIITOX. It has been an important starting point to structure toxicity characterisation models. **Fig. 6** shows an interpretation of the SETAC framework.

In the terminology of the SETAC framework the load, M, represents the amounts of substances emitted from the technical system. A substance emission model in LCA is equivalent to a model of the technical system in an LCI and M is

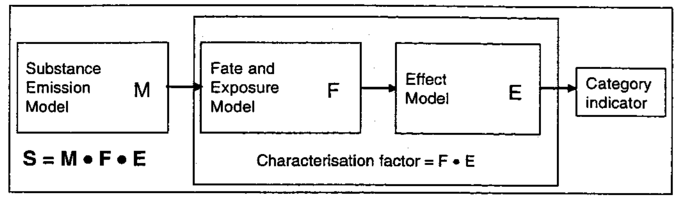

Fig. 6: General model framework for ecotoxicity and human toxicity characterisation within life cycle impact assessment according to SETAC Europe's First Working Group on Life Cycle impact assessment (WIA1) [7]. Arrows indicate cause effect chain causality

the LCI result. F is the exposure factor that is calculated by a fate and exposure model. The effect factor, E, is calculated by the effect model. The characterisation factor is an aggregation of the whole model into a single value per substance and emission scenario and is calculated by multiplying the exposure factor by the effect factor. The calculation of the impact score on the category indicator, S, is performed by multiplying the characterisation factor by the load.

When interpreting the SETAC framework with the terminology of the OMNIITOX concept model, three mechanism models can be distinguished: the fate and exposure model, the effect model and the overall characterisation model. The indicator of the effect model and the characterisation model are the same, i.e. the category indicator. The output from the exposure model must mathematically and contextually match the input to the effect model. The load of the fate and exposure model and the overall characterisation model is the same as the load concept, M, in the SETAC framework.

3.6 Support for consistent cause-effect chain modelling

The SETAC framework shows the possibility and the need to model cause-effect chains of the natural system. However, the structuring of a characterisation model does not necessary have to follow the SETAC structure where a fate and exposure model links to an effect model. Other approaches such as fate linking to exposure linking to toxic effect linking to economical cost etc. are equally valid. Therefore, the OMNIITOX concept model should provide the possibility to model an arbitrary number of cause-effect links. The key lies in the connectivity of the indicator of a mechanism with the load of the consequent mechanism.

In an industrial perspective we are concerned with how the technical system affects indicators in the natural system. In

Table 1: Core concepts of the OMNIITOX concept model and related concepts used in the contexts LCA, RA, and (eco)toxicology

OMNIITOX	Load	Indicator	Mechanism	Substance	Nature framework
Life cycle assessment	Environmental aspect, LCI result, inputs and outputs, emission, resource, load	Category indicator, midpoint, endpoint, damage	Environmental mechanism characterisation method, characterisation model	Substance, material, inputs and outputs name	System boundaries of characterisation method, receiving environment, landscape data
Risk assessment	Input, substance, chemical, stressor, dose	Risk, response, toxic effect	Dose-response model, fate exposure effect model	Chemical, substance, compound	Compartment, system boundaries
(Eco)Toxicology	Stressor, input, dose	Response, toxic effect	Dose-response model, exposure effect model	Chemical, substance, compound	Measurement conditions, laboratory set-up, compartment, system boundaries

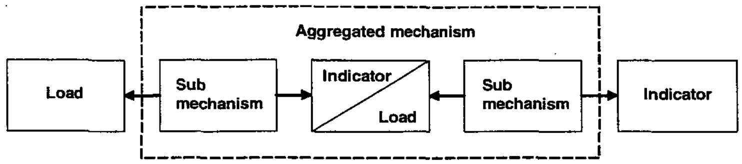

Fig. 7: A cause-effect chain can be modelled if the indicator of a mechanism is identical to the load of a subsequent mechanism. The aggregated mechanism encompassing sub-mechanisms can be regarded as a 'unit' mechanism. In this way, an arbitrary number of sub-levels of mechanisms may be modelled, documented, and communicated by using the OMNIITOX core concepts. Arrows indicate relational dependency

LCA, the emission and resource flows in an LCI result are an interface between the technical system and the natural system. For consistent use of LCI data in natural system models, a definition of a load that refers to technical systems flows should precisely match the information of this flow interface.

It is not necessary that a load originates from a technical system. The load may originate from any adjacent system of a mechanism, e.g. the load may refer to changes in environmental concentration that may be caused by natural mechanisms. This generalisation allows for the modelling of cause effect chains within the natural system with well-defined model inputs and outputs as shown in **Fig.** 7. In Fig. 7, the arrows indicate relational dependency. This gives that first the loads and indicators must be defined. Mechanisms are then defined as the relations between the loads and indicators.

In this sense a load is an indicator that can trigger mechanisms. In other words: a mechanism is the relation between indicators in the natural system. For example, an 'exposure and effect' mechanism model can describe the relation between the indicators 'concentration of nitrogen in water' and 'biomass of algae in water'[1]. Other mechanisms may describe the relation between 'biomass of algae in water' and 'biomass of fish in water', etc.

The interconnection of mechanisms, as shown in Fig. 7, implies a widening of the overall system boundaries, i.e. the connected sub-mechanisms are all members of a superior aggregated mechanism. If the inner sub-mechanism structure of the aggregated mechanism is disregarded, it is itself a 'unit' mechanism. The superior mechanism can in turn be incorporated as a sub-mechanism of yet another mechanism. In this way, an arbitrary number of sub-levels of mechanisms with different levels of detail and resolution can be transparently interconnected in the same model by using the same core concepts.

[1] To point out the generality of the cause-effect chain of load-mechanism-indicator the opposite relation is also feasible, i.e. the effect that 'biomass of algae in water' has on 'concentration of nitrogen in water' could be modelled.

To exemplify the indicator-load connectivity the OMNIITOX base model [2] is outlined in **Fig.** 8. The human impact mechanism is the relation between emissions from technical systems and two human toxic effect indicators. It encompasses a fate, an exposure, and an effect mechanism. The ecotoxicity impact mechanism is the relation between emissions from technical systems and one eco toxic effect indicator. Here the same fate mechanism as in the human impact mechanism is re-used and linked to an ecotoxicty effect mechanism.

4 Using the OMNIITOX Concept Model in LCA Characterisation Modelling

The concept model is compatible and interpretable with related established LCA concepts as defined in the ISO 14040 standards series [14–17]. In LCA a conceptual distinction between the concepts category indicator, and category endpoint [17] is made. In the OMNIITOX concept model these concepts are examples of indicators. Any indicator can be incorporated in an LCIA method by defining them as category indicators that can be weighted in accordance with LCA methodology.

The characterisation step can be mathematically expressed as a general characterisation function: CR=f(L, CP), where CR is the characterisation result i.e. the indicator value, CP are characterisation parameters, and L the LCI result, i.e. the load value. Here, the function f is the mechanism algorithm in its most aggregated form. The mechanism is the modelled physical representation that transparently explains the shape of the function f including all parameter derivations, assumptions, simplifications, and data aggregations modelled. The calculation of the characterisation parameters generally follows CP=f(S,N) where S are the required substance property values and N are the required nature property values. Characterisation factors (CFs) are a specific case of characterisation parameters. If CFs are applied, the mechanism describes a direct proportional relation between load and indicator: $CR = L \cdot CF$.

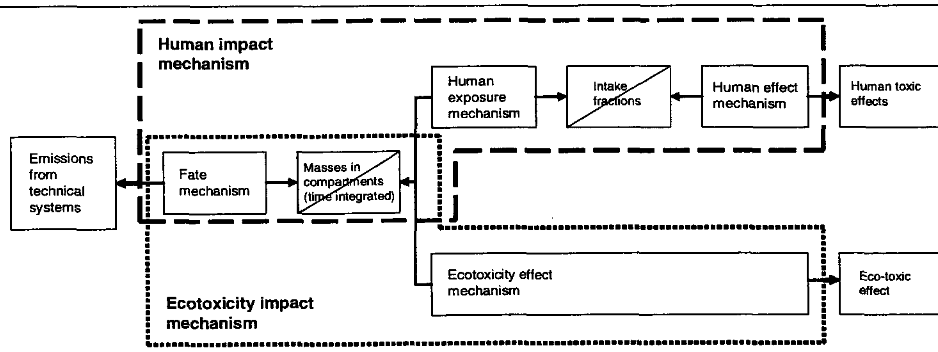

Fig. 8: The OMNIITOX base model outlined in terms of loads, mechanisms, and indicators. Arrows indicate relational dependency

When numerically comparing models, it is necessary to be clear about differences in loads and indicators between models. If they are in any way different, numerical differences in calculated characterisation parameters can be expected.

4.1 Usage and implementation of operational models

In order to create operational models and industrial tools an important requirement is to make it possible to easily extract the information relevant for usage of these often very complex models, i.e. it should be easy to understand how to apply a model and to assess the applicability of a model for a specific study. It is a simple task to assess how a characterisation model documented according to the OMNIITOX concept model should be applied in an LCA context. The load is a precise definition of what LCI data categories are applicable to the model. Any indicator referred by the mechanism can be defined as a category indicator. The nature framework gives the user an explanation of system boundaries that can be compared with the scope of the specific LCA study.

If the load, indicator, and mechanism algorithm of a model is unambiguously defined, it can be translated into well formatted data and software code by programmers and implemented on a computer. Upon implementation of the OMNIITOX characterisation models this structure has been used as a tool to assess model completeness and consistency.

5 Conclusions

The OMNIITOX concept model has been developed in a consensus based process by participants from the LCA, RA, and informatics disciplines.

The SETAC framework for ecotoxicity and human toxicity characterisation within life cycle impact assessment has been a starting point for the design of the OMNIITOX concept model. A characterisation model following the design of the SETAC framework can be easily interpreted into the OMIINTOX concept model. However, the OMNIITOX concept model has a higher level of flexibility and can be regarded as a generalisation of the SETAC framework to allow for scalability and arbitrary structure of cause-effect chain models.

The OMNIITOX concept model is compatible and interpretable with related established LCA concepts as defined in the ISO 14040 standards' series. Load definitions referring to technical systems specify the applicable data categories of the characterisation model. A category indicator is an indicator applied in an LCIA method, characterisation is the relation between an LCI result and a category indicator, which is identical to a mechanism that describes the relation between a load and an indicator and has system boundaries defined as a nature framework.

From a user perspective the OMNIITOX concept model facilitates the understanding of applicability, usage and interpretation of model output. Thus, the OMNIITOX concept model provides a common format for documenting, storing, reporting, and exchanging information in the multidisciplinary environment within the scope of OMNIITOX.

6 Outlook

In the further work with the implementation of the OMNIITOX IS the OMNIITOX concept model will describe all pieces of information in the OMNIITOX database. The database is at the heart of the OMNIITOX information system, and the fields and tables of the OMNIITOX database are directly derived from the OMNIITOX concept model, which makes it possible to have the same understanding of the data regardless of user perspective. It is a crucial support for data quality management within the OMNIITOX IS.

Though the scope of OMNIITOX only covers eco and human toxicity, the OMNIITOX concept model is designed to be applicable to any characterisation model. In addition, as the OMNIITOX concept model is created in a consensus process with participants from the LCA, RA, and toxicology disciplines, it is possible to use the OMNIITOX concept model as a tool in RA and toxicity modelling.

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